Spent Nuclear Fuel Analyses based on In-Core Fuel Management Calculations

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A method for performing spent nuclear fuel (SNF) analyses using in-core fuel management (ICFM) calculations has been developed and validated as described in this paper. Parameters such as decay heat, neutron source rates and photon spectra of discharged LWR fuel assemblies are calculated on the basis of ICFM core tracking data. This approach offers highly automated and accurate SNF analyses and eliminates the need for special fuel irradiation calculations to obtain the radiation source terms. This new SNF method has been validated against LWR spent fuel isotopic measurements, by comparisons with ORIGEN-ARP calculations and comparisons with a decay heat standard. A further validation effort against experimental decay heat data from a Swedish fuel storage facility is underway.

KEYWORDS: Spent nuclear fuel, radiation source terms, decay heat, in-core fuel management.

1. Introduction

Knowing the isotopic contents in the fuel at the time of discharge from the reactor is a prerequisite for back-end fuel cycle calculations with applications to storage, transportation and disposal of spent fuel. Solving the isotopic decay chains and using the summation method to calculate the radiation sources, these may be calculated at any time after discharge. The ENDF/B-VI and JEF-2.2 data libraries of CASMO-4 and HELIOS include a large number of actinides and fission products that are individually represented and tracked per fuel pin in ordinary ICFM fuel depletion calculations [1], [2]. By a careful selection of isotopes included in the summation it is possible to obtain high accuracy. It was found that in addition to the lattice code library isotopes, several other isotopes have to be taken into account in SNF calculations. Thus several fission products daughter isotopes, lower isotopes of the actinides decay chains and structural material activation products have also been included. In general, the number of fission product isotopes required to obtain a given accuracy increases with decreasing cooling time and hence special care must be taken for cooling times less than e.g. a few days as described below.

The operating history of a given fuel assembly is obtained from the ICFM 3-D simulation, e.g. using SIMULATE-3 core tracking calculations [3]. The isotopic concentrations to be used in the SNF calculation are thus evaluated on a nodal level, based on the final burnup, spectrum history and power density history of each axial node of a given fuel assembly. The residual heat and radiation source terms are calculated by summation of the isotope-wise contributions of the released energy, neutron yields and photon release rates. The required library data were obtained from the ENDF/B-VI Decay Data File [4], supplemented with e.g. neutron yield data from JAERI [5].
2. Methods of calculation

The SNF method includes calculation of radioactivity, decay heat, gamma heat, spontaneous fission and \((\alpha, n)\)-reaction source neutrons as well as photon release rates and spectra. The photon spectrum is calculated in 18 energy groups based on decay gammas and x-ray data from the ENDF/B-VI file and including also models for photons associated with spontaneous fission and \((\alpha, n)\)-reactions of actinides and bremsstrahlung from the most important \(\beta\) – emitters. The concentrations of special isotopes of importance in e.g. safeguards, burnup credit, etc., may be edited if desired. Utilizing the ICFM core tracking data and results, the SNF analysis of a given fuel assembly at a given cooling time is highly automated and may be performed as ‘post-processing’ of the standard core tracking calculations.

The simplifying assumptions usually employed in traditional spent fuel calculations, such as the lack of detailed 2-D lattice physics and a coarse modeling of the power density history, are avoided [6]. The CASMO-4 isotopic concentrations are tabulated vs. burnup and spectrum history parameters in the same way as cross sections and other parameters needed by the 3-D simulator model. The actual, nodal concentrations at the time of discharge are obtained by interpolation using the final, nodal burnups and history parameter values and applying a special correction accounting for the power density history of the node. The power density history typically consists of several hundred time-steps representing the core tracking burnup-steps and shutdown periods. The power history correction factor, \(c_{\text{ph}}\), of an isotope, \(j\), is here defined as:

\[
c_{\text{ph}} = \frac{C_{\text{actual}}^j}{C_{\text{ref}}^j}
\]

where the final concentrations \(C_{\text{actual}}^j\) and \(C_{\text{ref}}^j\) are computed by suitable approximations of the isotopic depletion/build-up chains of the isotope considered, using the actual power density history from the 3-D simulation and the reference power density of the 2-D lattice code calculation, respectively. For fission products with relatively short half-lives and low neutron absorption, the change in the concentration, \(C^j\), during a time step, \(\Delta t\), is defined as:

\[
\Delta C^j = \mu^j \cdot F(1 - e^{\lambda^j \Delta t})
\]

where \(\mu^j\) and \(\lambda^j\) are the fission yield and decay constant of the isotope, respectively, and \(F\) is the fission rate which is assumed proportional to the nodal power density. A similar, but more complex approximation, is used for fission product daughter isotopes. Some important actinides, e.g. Cm-242, are also quite sensitive to the power density history. In fact, several actinides depletion/build-up chains have to be modeled in detail to properly calculate the history correction factors of the most important actinides. Examples of SNF history correction factors of Cm-242 in comparison with those of the fission product Ce-144 are shown in Fig. 1. This illustration concerns a test case with a five-step power history with relative powers of 1.0, 0.5, 2.0, 0.5 and 1.0 as shown in the figure. The reference results for this test were generated by a HELIOS calculation.
Fig. 1 Power history correction factors vs. burnup for a step-wise variable power test case (SNF) in comparison with reference results using the lattice code depletion/build-up chains.

The actinide decay chains have been extended relative to those of CASMO-4 and HELIOS. An example is the inclusion of the Rn222 -> Pb210 chain consisting of eight actinides that only are of interest at very long cooling times (e.g. 10,000 years). Another example is the Pu236 -> Tl208 chain, which was included due to the high-energy gammas emitted by Tl208. The elements Fe, Ni, Co, N and Cl have also been included in the SNF model to account for radiation due to Fe-55, Ni-59, Ni-63, Co-60, C-14 and Cl-36. The radiation source terms are readily calculated from the decayed isotopic concentrations using the library data described above.

Application of the summation method for very short cooling times (1 sec – a few days) would require modeling of a large number of short-lived fission products that are not represented in ICFM codes and libraries. Instead, the ANS-5.1-1994 Decay Heat Standard [7] is utilized to obtain the total or ‘lumped’ decay heat of the short-lived fission products. This is achieved by separating the modeling of the last three days of the operating history from the remaining history. The ANS-5.1 Standard is then used to calculated the fission product decay heat resulting from the final, three-days period whereas that due to the remaining history is calculated by the summation method. As opposed to the short-lived fission products, all the important short-lived actinides are included in the SNF model and thus the summation method is always valid for these isotopes, independently of the cooling time. This assures e.g. accurate neutron source calculations, even for cooling times in the order of seconds. An illustration of the contributions to the total decay heat from the lumped fission products, the explicitly represented fission products and the actinides is shown in Fig. 2.

3. Validation

The SNF method described above has been implemented as a calculation module called SNF interfacing with Studsvik Scandpower’s ICFM codes, using either CASMO-4 or HELIOS for generation of the required isotopic data tables. The validation basis of these codes includes numerous isotopics comparisons with experimental data. The recent JAERI spent fuel isotopic measurements [8] have been
analyzed with CASMO-4 using the JEF-2.2 library in connection with the SNF development. More than 40 nuclides of uranium, transuranium, and fission products were measured in BWR and PWR fuel samples with burnups up to about 47 GWd/t.

![Graph showing decay heat and contributions](image)

**Fig. 2** Total decay heat and contributions from lumped fission products (F.P.- lumped), explicit fission products (F.P.- summation) and actinides for short cooling times. Typical BWR fuel at 30,000 MWd/t discharge burnup.

A summary of the isotope-wise average C/E values of 29 samples of PWR rods SF95, SF97 and BWR rods SF98 and SF99 is shown in Figs. 3 (actinides) and 4 (fission products). The isotopes from U-235 to Am-241, show quite good agreement, although Np-237 and Pu-238 are under predicted by about 9%. The higher isotopes, from Am-242m to Cm-246 and the curium isotopes are under predicted typically about 20%. The quoted experimental uncertainties of most of the actinides are small (0.1 - 2%), except for those of Am-242m, Cm242 and Np237 (<10 %). The reason for the observed under prediction is not known, however, it is interesting to note that Japanese authors have reported similar under predictions of these isotopes using the SWAT code and the JENDL-3.2 nuclear data library [9]. The fission product isotopes of neodymium, cesium, cerium and samarium all show good agreement.

The isotopic decay and source terms calculations, starting from a given set of isotopic concentrations at the time of discharge, has been validated by comparison of SNF results with a number of ORIGEN-ARP [10] calculations for typical BWR and PWR fuel samples. First, a set of ORIGEN-ARP irradiation+decay calculations was performed to generate the reference results (with all ORIGEN-ARP library isotopes present). Then, the concentrations at discharge of the isotopes represented in the SNF code were copied from the ORIGEN-ARP output and used as initial concentrations for decay and source terms calculations with the SNF code. An example of %-differences between such SNF and ORIGEN-ARP calculations of activity, decay heat, neutron source rates and photon source rates for a BWR case is shown in Table 1. All parameters agree within 0.3% for cooling times up to 10,000 years. The same accuracy was obtained for corresponding PWR calculations. The results are considered very satisfactory, considering that the number of isotopes included in the SNF calculation is much less than...
that of ORIGEN-ARP.

**Fig. 3** CASMO-4 vs. the JAERI spent fuel benchmark – average C/E values for actinides

**Fig. 4** CASMO-4 vs. the JAERI spent fuel benchmark – average C/E values for fission products
Table 1 Differences in percent between SNF and ORIGEN-ARP calculations of activity, decay heat, neutron source rates and photon source rates for discharged BWR fuel.

<table>
<thead>
<tr>
<th>Discharge burnup (MWd/t)</th>
<th>Cooling time (years)</th>
<th>Activity (%)</th>
<th>Decay heat (%)</th>
<th>Neutron source (%)</th>
<th>Photon source (%)</th>
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A comparison of SNF calculation of the fission product decay heat with that obtained using the ANS-5.1-1994 Decay Heat Standard is shown in Fig. 5. The cooling time range is 1 - 10^{10} sec (about 300 years), which is the range of validity of the ANS Standard. The calculation concerns a BWR fuel sample at 30,000 MWd/t. The agreement is within 1 % for cooling times up to 30 years, except around 3 years where a slightly larger discrepancy was found. The ‘neutron capture correction’ of the ANS Standard, which is difficult to determine, has its maximum value around 3 years cooling time and may explain the larger discrepancies at these cooling times. At 300 years, where the fission product decay heat is only about 1 W/t, the SNF value was about 0.1 W/t higher than the Standard. However, the overall agreement is regarded as good, considering the large span in the calculated decay heat (from 1 to 10^{6} W/t).

An ORIGEN-ARP calculation of the fissions products decay heat for short cooling times was also carried out. The result fell about 4 % below that of the Standard at 1 sec but increased to a level about 1 % above the Standard at 10^{4} sec. The capability of the SNF program to calculate the decay heat for short cooling times and combined with the nodal modeling may be utilized e.g. to accurately calculate the core thermal power following shutdown, etc.

An experimental program for measuring the decay heat of spent PWR and BWR fuel assemblies stored in the CLAB facility in Sweden is presently performed by the Swedish company SKB in collaboration with ORNL [11]. Studsvik Scandpower performs an evaluation of SNF against these
measurements in cooperation with the Swedish nuclear utilities, using their CASMO-4/SIMULATE-3 ICFM core tracking models. This effort will add new data to the validation base of the SNF method described in this paper.

![Graph showing comparison of SNF fission products decay heat with the ANS-5.1 Standard](image)

**Fig. 5** Comparison of SNF fission products decay heat with the ANS-5.1 Standard

### 4. Conclusion

A method has been described for calculation of spent nuclear fuel source terms, such as activity, decay heat, and neutron and photon sources, based on ICFM core tracking codes. In particular, the following conclusions were made:

- The limitations of traditional spent fuel codes concerning lattice heterogeneities (e.g. of BWR assemblies), burnup, neutron spectrum representation, etc. are avoided.
- The number of isotopes represented in the recent ENDF/B-VI and JEF-2.2 libraries of CASMO-4 and HELIOS is sufficient for spent fuel source terms calculations using the summation method.
- The ANS-5.1 Decay Heat Standard may be utilized to calculate the decay heat due to short-lived fission products not included in the lattice code libraries in calculation cases with very short cooling times.
- The influence of the detailed operating history and neutron spectra on the isotopic contents of discharged fuel assemblies is obtained from ICFM core tracking calculations and thus the isotopic concentrations are calculated in each axial node of the fuel assemblies.

The validation of the ICFM/SNF method shows that:

- The calculated isotopic concentrations in spent fuel agree well with experimental data.
- The calculated source terms and residual heat are in good agreement with ORIGEN-ARP calculations and with the ANS-5.1-1994 Decay Heat Standard.
References